

Practical work on Molecular Dynamics: Toughness of a notched nano-specimen

Master program DMS

February 17, 2025

1 Introduction

In this practical work we will compute toughness of a notched nano-specimen by means of molecular dynamic (MD) simulations. The simulations will be carried out in one of the most popular open-source MD softwares [LAMMPS](#) from Sandia National Laboratories. Toughness of a material characterizes the amount of energy per volume needed to rupture it and can be computed by integrating the work done on the specimen to rupture it. For the simplest case of brittle rupture in tension of a bar of section A and length L (i.e. the volume is $V = AL$), the work of a force F until its rupture at $F_r = EAu_r/L$, where E is the material Young's modulus. The work done by the force is

$$W_r = \int_0^{u_r} F(u)du = \frac{EAu_r^2}{2L} = \frac{F_r^2 L}{2EA} = \frac{\sigma_r^2 AL}{2E},$$

where σ_r is the critical stress. By dividing this energy by the volume, we obtain material toughness

$$G = \frac{W_r}{LA} = \frac{F_r^2}{2EA^2} = \frac{\sigma_r^2}{2E}$$

Therefore in brittle materials the toughness is exclusively determined by the critical stress σ_r and Young's modulus E . In ductile or quasi-brittle materials, fracture is accompanied with energy dissipation either by plastic slip (dislocations glide) or by damage accumulation (micro-cracks, micro-pores, voids, etc). Therefore, for such materials, their toughness can be higher than if the material would behave in purely brittle way. The dissipative processes is generally localized in front of the crack tip and it forms a so-called process zone. Simply speaking, the more energy is dissipated in fracture, i.e. the higher the toughness, the "harder" the material is to break.

To study the material toughness, we will use 2D molecular dynamics simulations of a notched or smooth specimen in uniaxial traction (Fig. 1). The objective is to understand a link between material toughness and initial porosity as well as with parameters of Lennard-Jones pair potential, loading rate, and, if time permits, with lattice orientation.

2 Set-up

The set-up is depicted in Fig. 1 and consists of a dog-bone type specimen with a wide zone for "grips" and a thinner zone where a uniform stress distribution is ensured. The input file is made parametrizable, so than one can control the width W and the height H of the specimen as well as the curvature radius r of the transition zone. In addition, the specimen contains some porosity and can have a notch or double notch (two symmetric notches located on both sides). The motion of atoms in the upper and lower zones (shaded in yellow in the figure) is restricted. A linear initial distribution of vertical velocities is applied through the specimen so that the lower side remains fixed and the upper moves vertically at speed V with a linear distribution in between. On the upper and lower side the vertical force is measured as well as the displacement of the upper part and is saved in the log file.

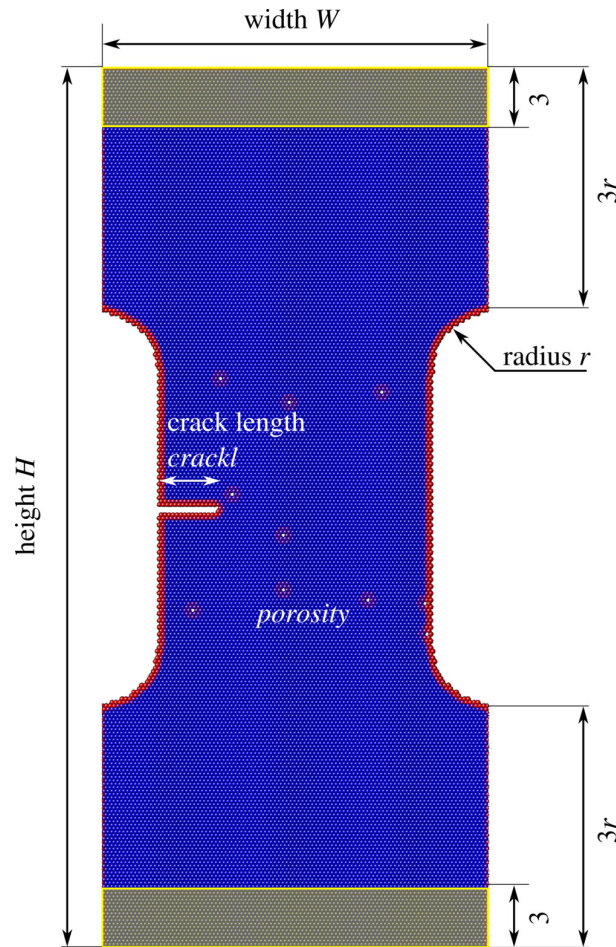


Figure 1: Specimen geometry and problem set-up.

3 Provided files

To download all necessary files, go to www.yastrebov.fr/TPMD2023.zip.

1. [in.tension](#): input file for LAMMPS MD simulations with comments.
2. [compute_area.py](#) : a python script to compute the work of the force and to plot force-displacement curve.
3. [README](#): a text file with useful commands.
4. [TP_MD_CRACK_2023.pdf](#) this document.

4 How to start?

To execute simulation, type in terminal:

```
$ lmp -var t 1000 -in in.tension
```

It will produce a log file [log.lammps](#) and few images. You can open them by typing

```
$ eog neighbours_image.0.jpg
```

Now, let's make a new geometry. To do so, open input file

```
$ gedit in.tension
```

and specify needed width **variable W**, height **variable H** and curvature radius **variable r**. Run the simulation again:

```
$ lmp -var t 100 -in in.tension
```

and check your geometry

```
$ eog neighbours_image.0.jpg
```

All other parameters which could be specified by the user are marked with **# USER DEFINED**, namely:

- **V**: loading rate
- **T**: temperature
- **W**: specimen width
- **H**: specimen height
- **epsilon**: bonding energy in Lennard-Jones 6-12 potential ϵ
- **r**: curvature radius of the dog-bone specimen
- **porosity**: porosity of the material
- **seed**: seed for random number generator to distribute pores in the material
- **crackl**: length of the notch
- **twocracks**: (boolean: true/false) determines if two notches are inserted

In the input file **in.tension** all explanations are provided. LAMMPS documentation can be found here lammps.sandia.gov/doc/Manual.html.

5 Study of toughness

To estimate toughness we measure displacement and force on the upper “grip”. These parameters are stored in the log file, which could be later read by a Python script **compute_area.py**. Prescribe a loading rate **V** and run simulation (without notches) on a longer time, for example:

```
$ lmp -var t 30000 -in in.tension
```

Ensure that the specimen was completely broken at the end of the simulation (check images). Now to construct a force-displacement curve and to estimate its integral, i.e. the work done to rupture the specimen, one can run a specifically prepared script:

```
$ ./compute_area.py log.lammps
```

this script reads stored data, store them separately in file **force_displacement_log.data** and makes a plot **Force_displacement.png** with indicated work (its value is also indicated in the screen). Determine the toughness which is nothing but this work divided by the specimen area.

Your objective is now to study how the following parameters influence the toughness:

- Make a series of simulations without notches with different **porosity** (do not go beyond 10%); make several simulations for every value of porosity by changing **seed** to get statistically meaningful data.
- For a selected porosity, study the influence of **epsilon** parameter (which represents the bonding energy between atoms) on the toughness and on the type of force-displacement curve. Do not use notches. To compare obtained values, normalize the toughness by **epsilon** parameter. For every **epsilon**, make few simulations to get statistically meaningful data.
- Make a series of simulations of crack propagation for different values **epsilon**. Sample simulation results are shown in Fig. 2.

At the same time, the effect of loading rate **V** and temperature **T** could be studied. If the time permits, one can study the effect if different crystal orientations, which can be set in **lattice ...orient**.

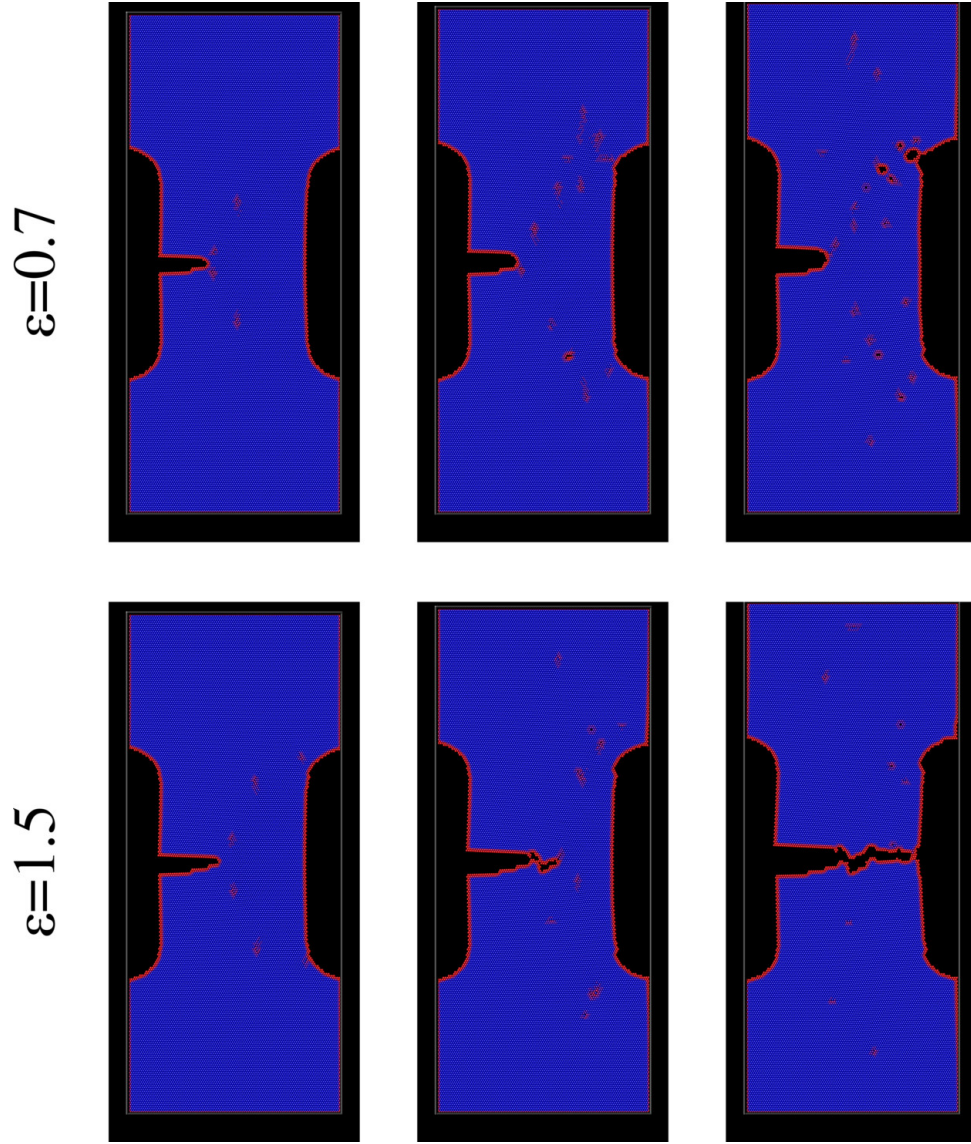


Figure 2: Snapshots of fracture simulation for different bonding energy ε for perfect crystal (no initial porosity) shown for the same time moments. The red defects in the lattice correspond either to pores or to dislocations.

6 Numerical data

Examples of values of LJ-6-12 parameters for some metals

- Nickel (Ni): $\sigma = 1.5808 \text{ \AA}$ and $\varepsilon = 0.1729 \text{ eV}$
- Chromium (Cr): $\sigma = 2.7812 \text{ \AA}$ and $\varepsilon = 0.24322 \text{ eV}$

7 Questions for the evaluation

Please prepare a short report in the format of your choice. A correct and complete answer for each question adds you one point, thus your note is $N \in [0,4]$.

0. Your name¹:

1. Describe your simulation results with and without a notch.

2. How does the initial porosity influence the stress/strain curve? What is the variability of this curve for different realizations (different [seed](#) used)?

3. How does the initial porosity influence the material toughness? Plot toughness change with respect to porosity change.

4. Describe crack propagation in the structure for different values of [epsilon](#). Explain your observations.

¹Sorry, for this question you do not get any points ☹.